

# A CAPE-OPEN Compliant Object for Large-scale Nonlinear Programming

**Yi-dong Lang and Lorenz T. Biegler**

Department of Chemical Engineering

Carnegie Mellon University

2<sup>nd</sup> Annual U.S. CAPE-OPEN Meeting

May 25, 2005 Morgantown, WV

# Outlines

- Introduction
- What is IPOPT
- Main features of IPOPT
- How to make IPOPT CAPE-OPEN compliant
- IPOPT with CO Tester
- Conclusions

|                        | MILP | MINLP | Global | LP,QP | NLP | SA/GA |
|------------------------|------|-------|--------|-------|-----|-------|
| HENS                   | X    | X     | X      | X     | X   | X     |
| MENS                   | X    | X     | X      | X     | X   | X     |
| Separations            | X    | X     |        |       |     |       |
| Reactors               |      | X     | X      | X     | X   |       |
| Equipment Design       |      | X     |        |       | X   | X     |
| Flowsheeting           |      | X     |        |       | X   |       |
| Scheduling             | X    | X     |        | X     |     | X     |
| Supply Chain           | X    | X     |        | X     |     |       |
| Real-time optimization |      |       |        | X     | X   |       |
| Linear MPC             |      |       |        | X     |     |       |
| Nonlinear MPC          |      |       | X      |       | X   |       |
| Hybrid                 | X    |       |        |       | X   |       |

# What is IPOPT

$$\min f(x, y)$$

$$\begin{aligned} s.t. \quad & g^L \leq g(x, y) \leq g^U \\ & x^L \leq x \leq x^U \\ & y^L \leq y \leq y^U \end{aligned}$$

MINLP

$$\min f(x)$$

$$\begin{aligned} s.t. \quad & g^L \leq g(x) \leq g^U \\ & x^L \leq x \leq x^U \end{aligned}$$

NLP

# IPOPT Strategies

$$\min f(x)$$

$$\begin{aligned} s.t. \quad & g^L \leq g(x) \leq g^U \\ & x^L \leq x \leq x^U \end{aligned}$$

$$\min f(z)$$

$$\begin{aligned} s.t. \quad & c(z) = 0 \\ & z^L \leq z \leq z^U \end{aligned}$$

$$\min \varphi(z) = f(x) + \mu \left\{ \sum \ln(z^U - z) + \sum \ln(z - z^L) \right\}$$

$$s.t. \quad c(z) = 0$$

# IPOPT Algorithm – Features

## *Line Search Strategies for Globalization*

- $\ell_2$  exact penalty merit function
- augmented Lagrangian merit function
- **Filter method (adapted and extended from Fletcher and Leyffer)**

## *Hessian Calculation*

- BFGS (full/LM and reduced space)
- SR1 (full/LM and reduced space)
- **Exact full Hessian (direct)**
- Exact reduced Hessian (direct)
- Preconditioned CG

## *Algorithmic Properties*

**Globally, superlinearly convergent** (Wächter and B., 2005)

Easily tailored to different problem structures

## *Freely Available*

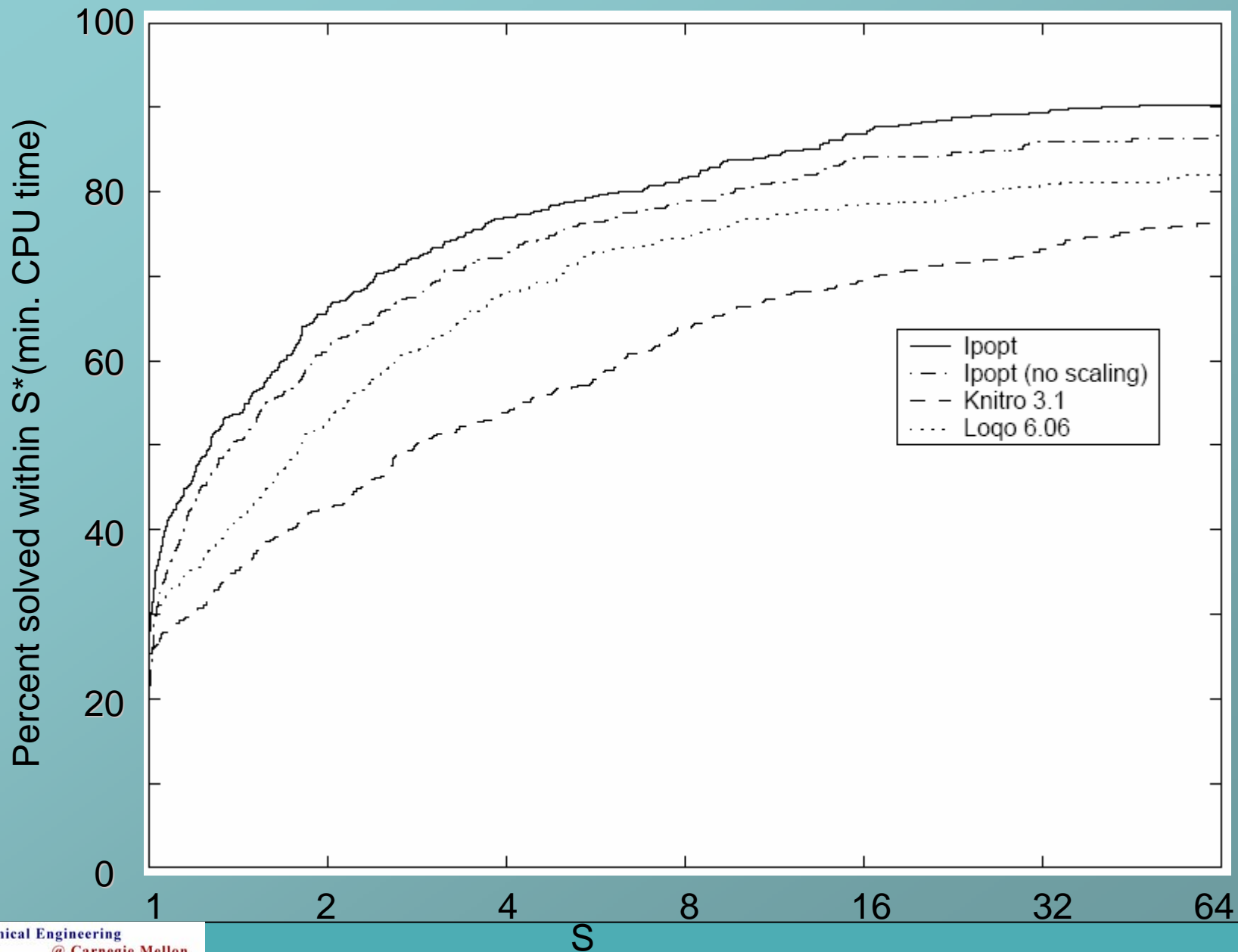
CPL License and COIN-OR distribution:

**<http://www.coin-or.org>**

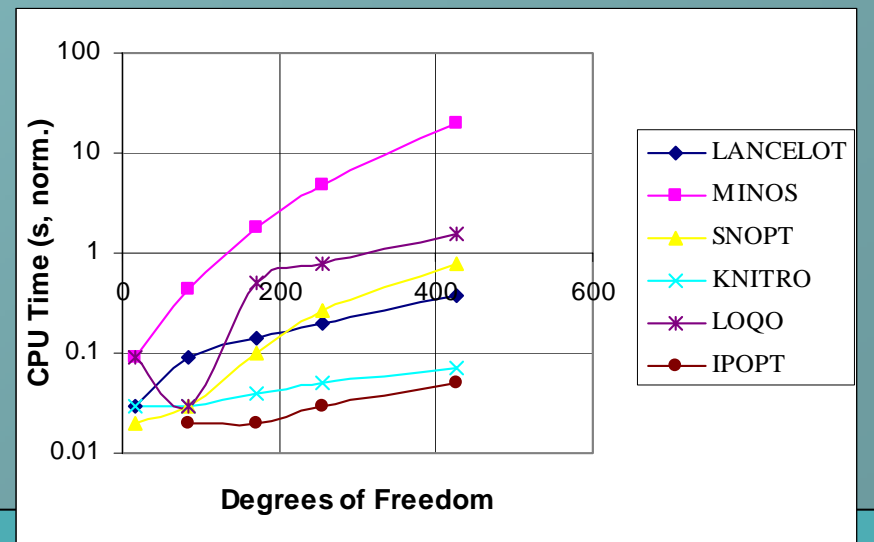
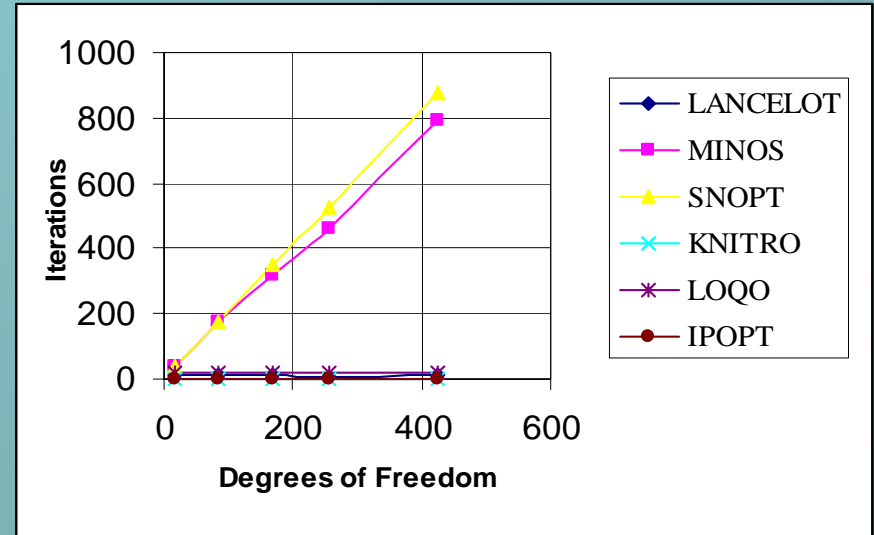
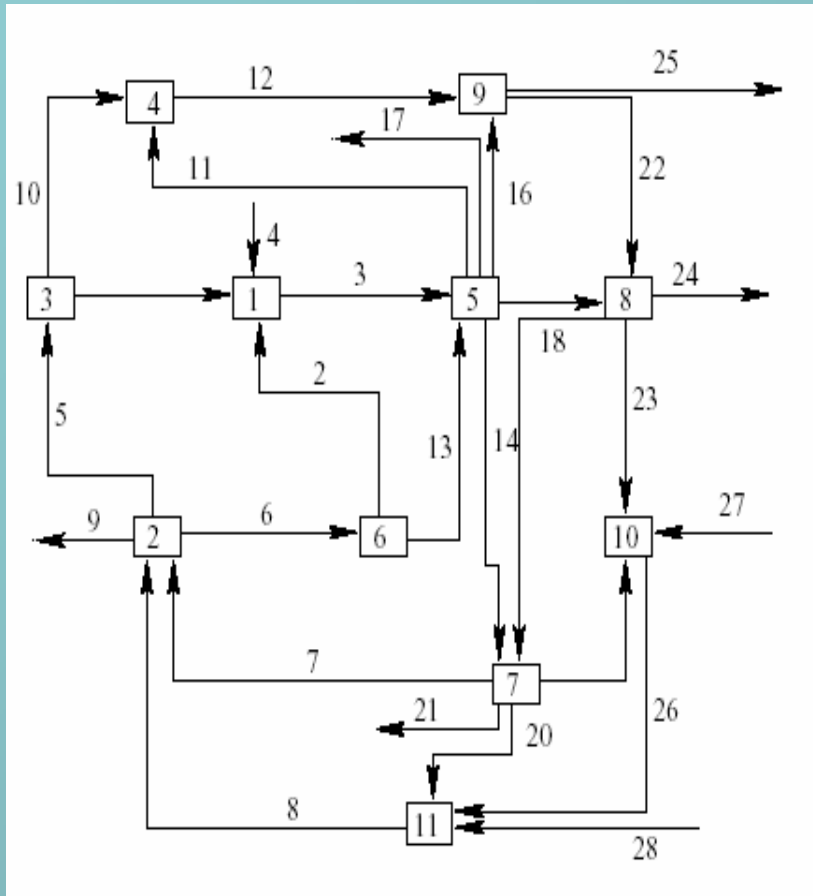
Beta version recently rewritten in C++

Solved on thousands of test problems and applications

# IPOPT Comparison on 954 Test Problems



# Comparison of NLP Solvers: Data Reconciliation



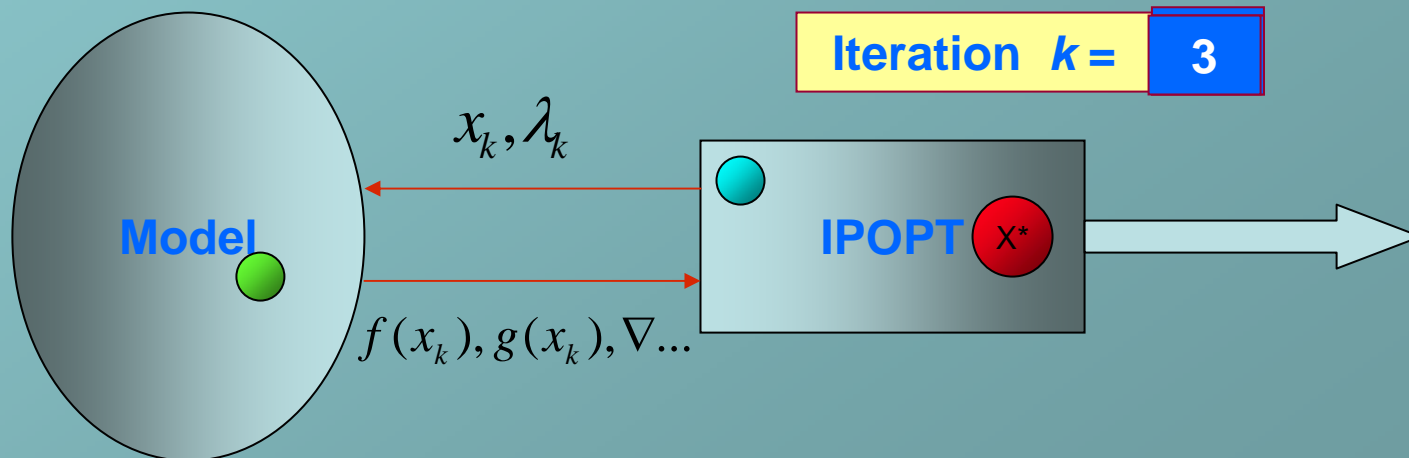


# Current Activities – IPOPT

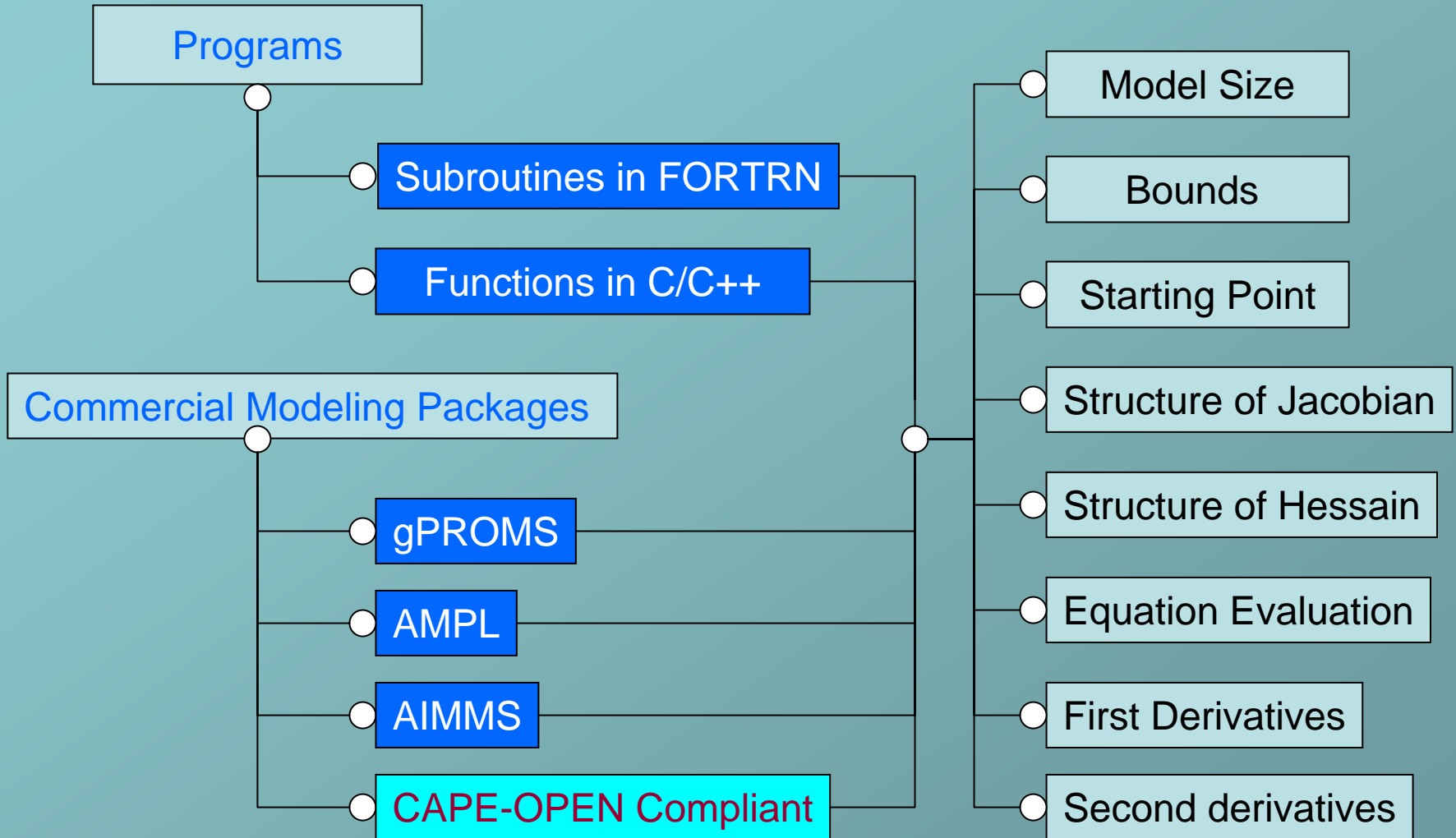
- Conversion of IPOPT from FORTRAN to C++
  - Modular - easier to maintain and modify
  - Interfaces to modeling packages and linear solvers
  - Parallelism for free
- IBM MINLP Project
  - Combine open source tools (e.g., CBC, IPOPT) to build state-of-art MINLP solvers
- Interfaces to Modeling Environments
  - AMPL – widely used
  - ROMeo – done
  - AIMMS – done
  - CAPE-OPEN – done

# Information & Its Flow

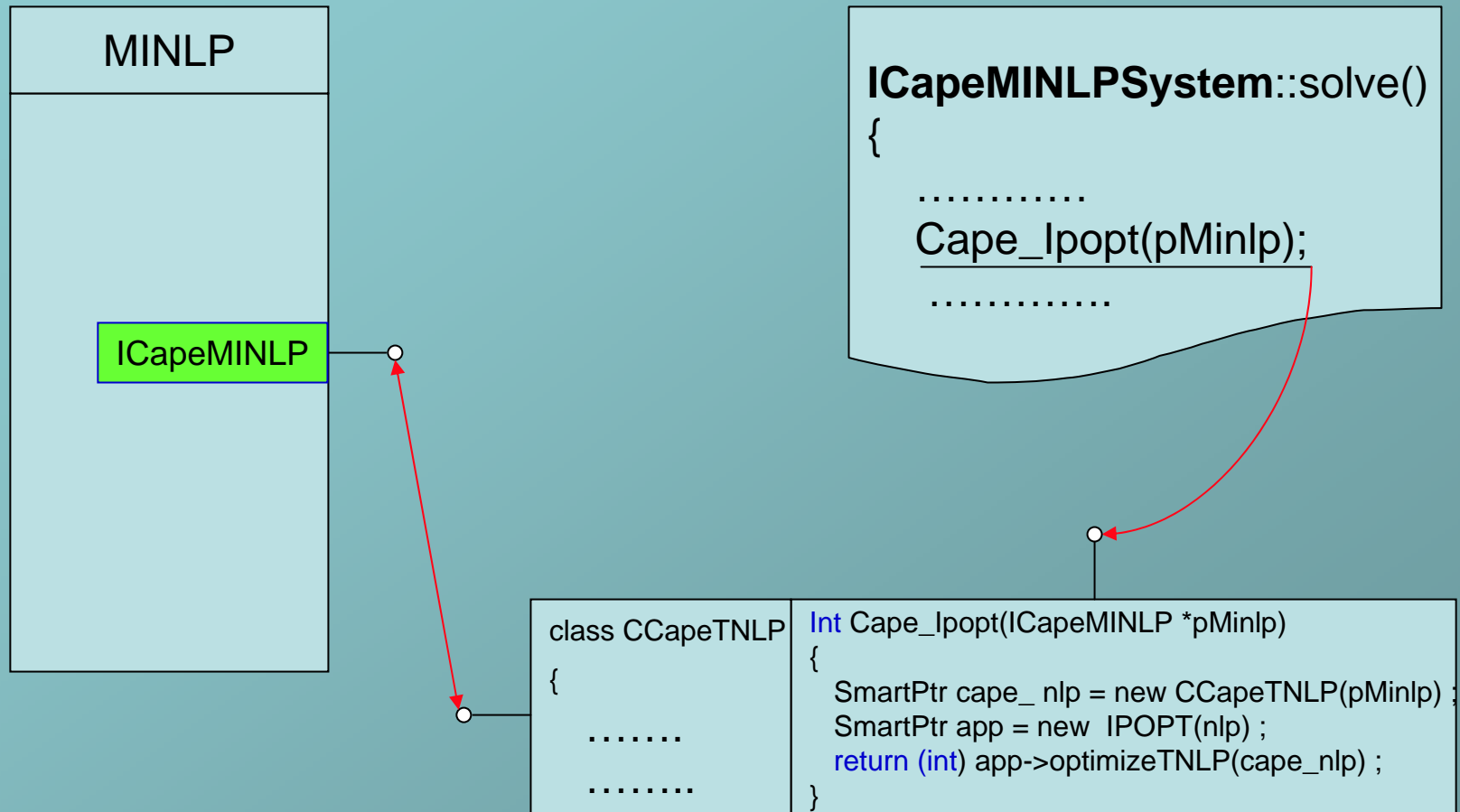
$$\begin{bmatrix} W_k + \Sigma_k & A_k \\ A_k^T & 0 \end{bmatrix} \begin{bmatrix} \Delta z_k \\ \lambda_k \end{bmatrix} = - \begin{bmatrix} \nabla \varphi(z_k) \\ c(z_k) \end{bmatrix}$$

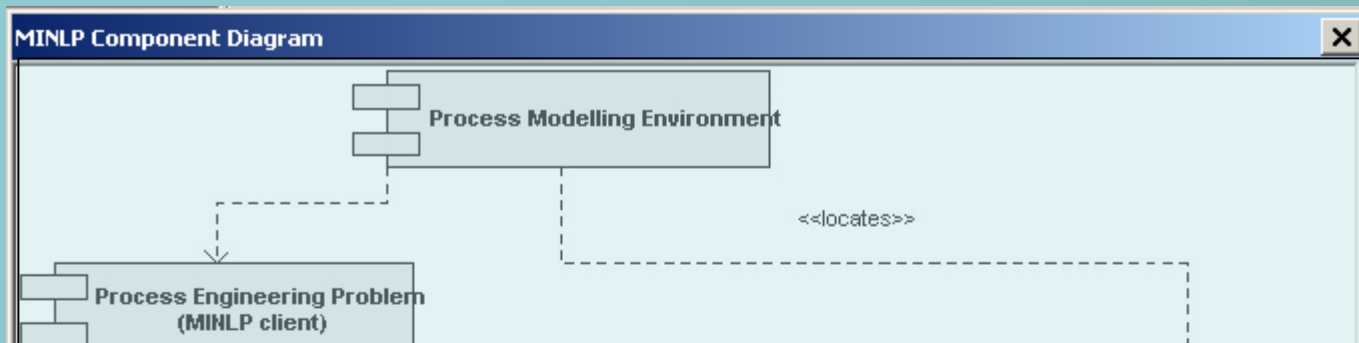


# How to Get Model

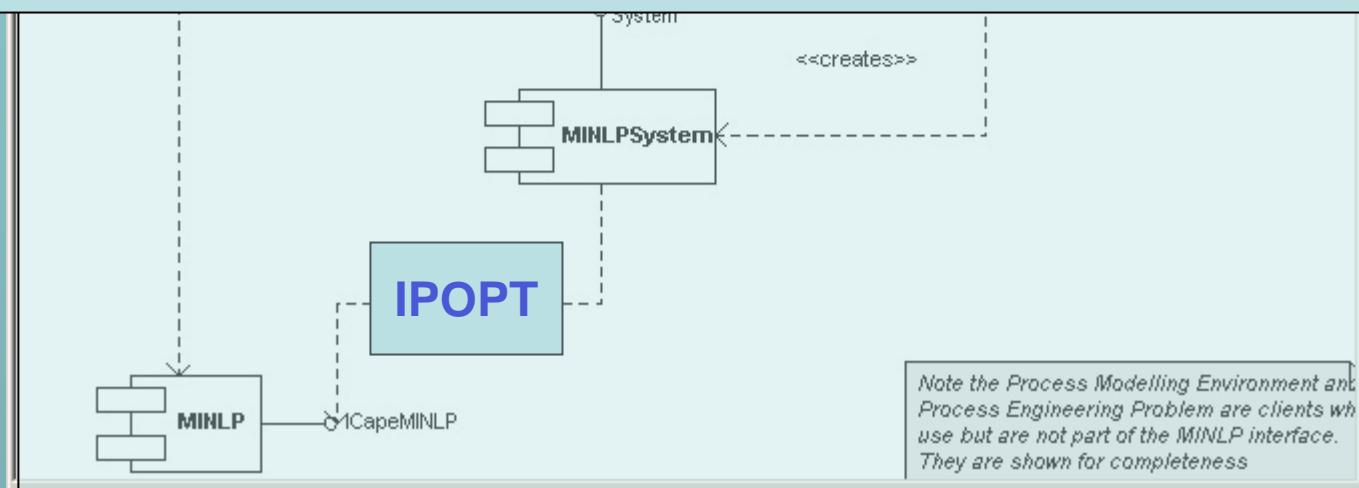


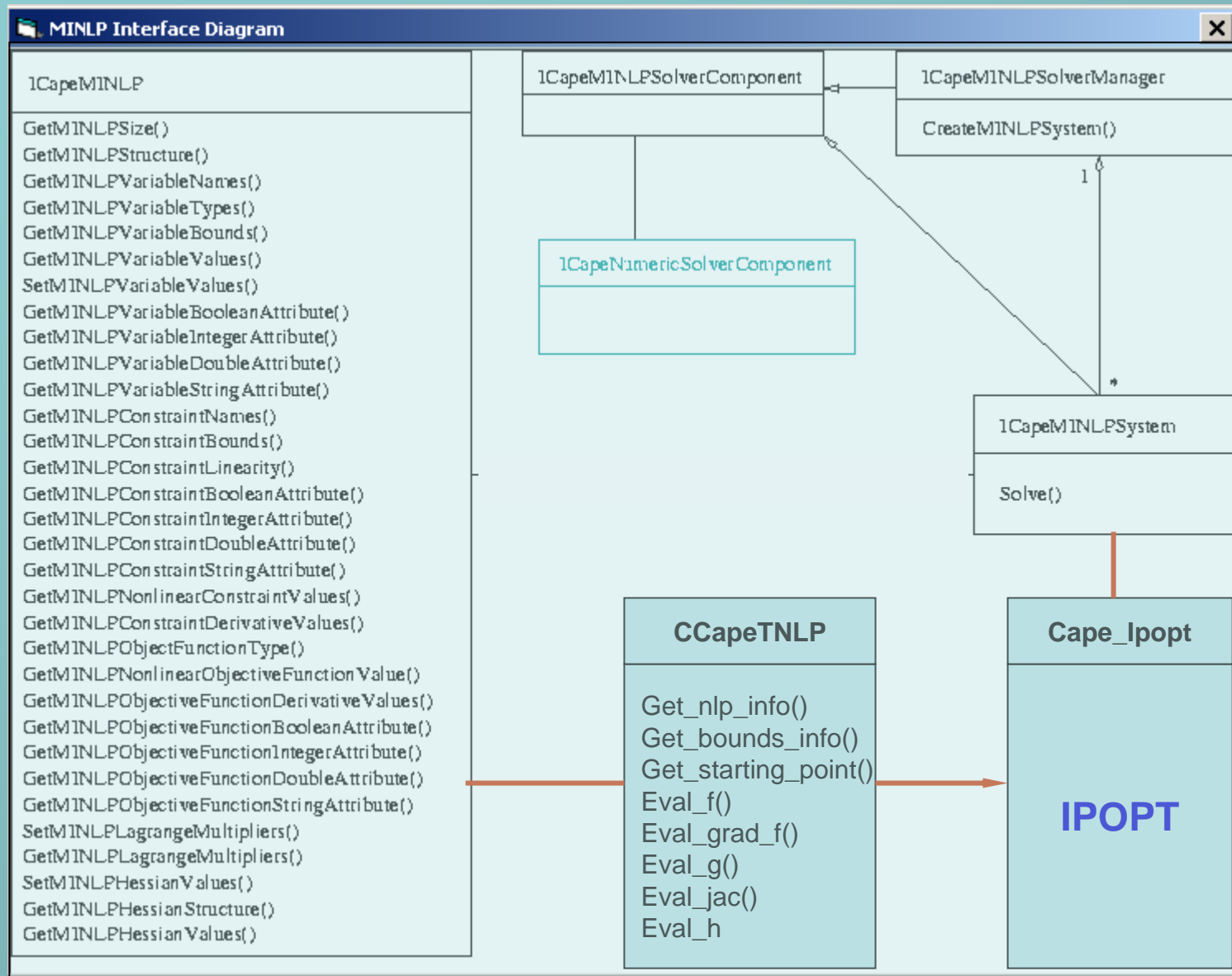
# CAPE-OPEN Compliant



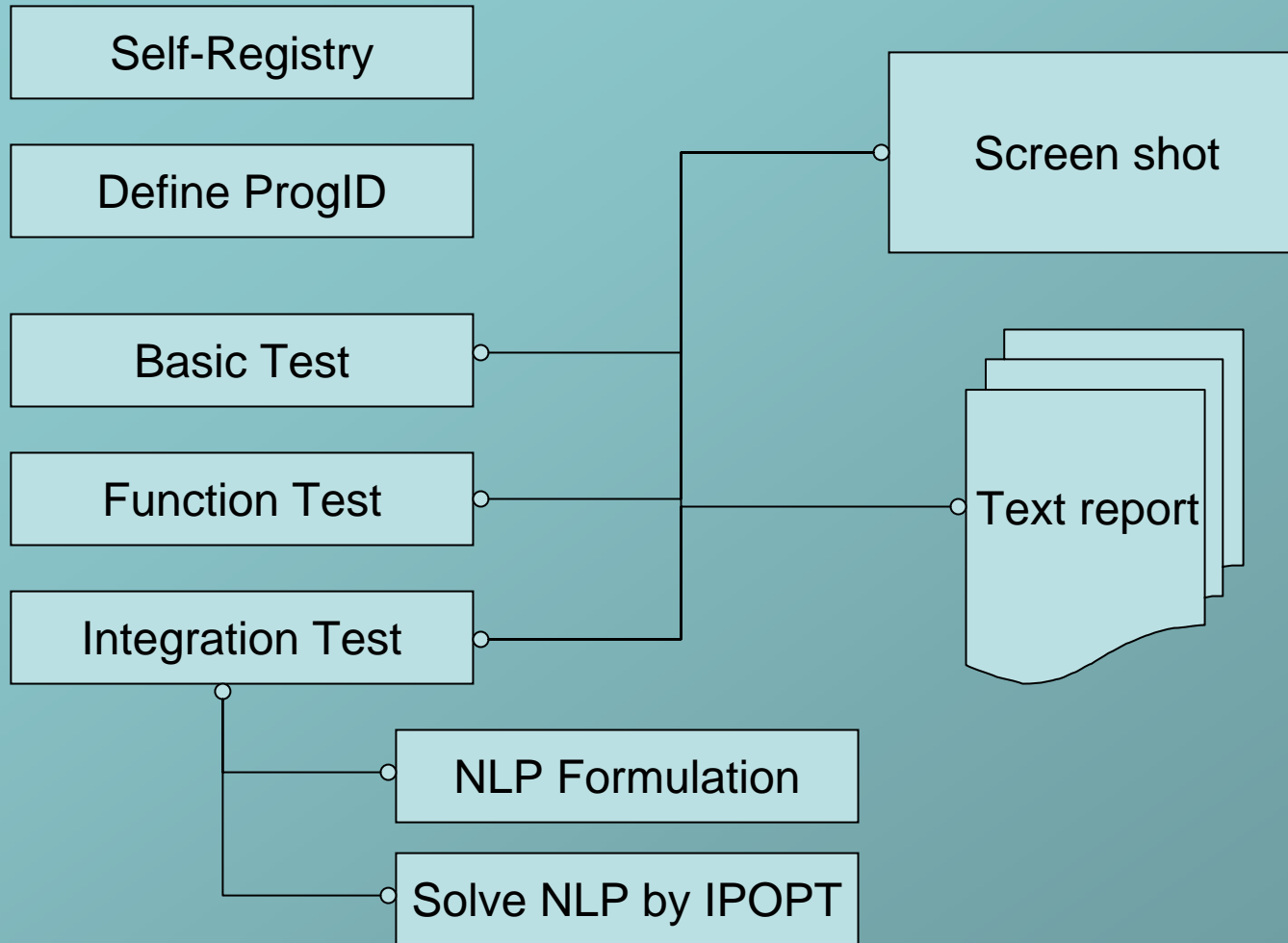


# Position of IPOPT in MINLP





# IPOPT & CO Tester



# Test with an Example

## NLP Formulation

MINLP Problem Creation - C:\Documents and Settings\Yidong\My Documents\My DATA\CAPE-OPEN\From Michel\Tester\CO...

|    | X1 | X2 | X3 | Y1 | Y2 | Y3 | Log(X2+1) | Log(X1-X2+) | Constant | Type |
|----|----|----|----|----|----|----|-----------|-------------|----------|------|
| OF | 0  | 0  | -7 | 5  | 6  | 7  | 18.0      | 19.2        | 10       | Min  |

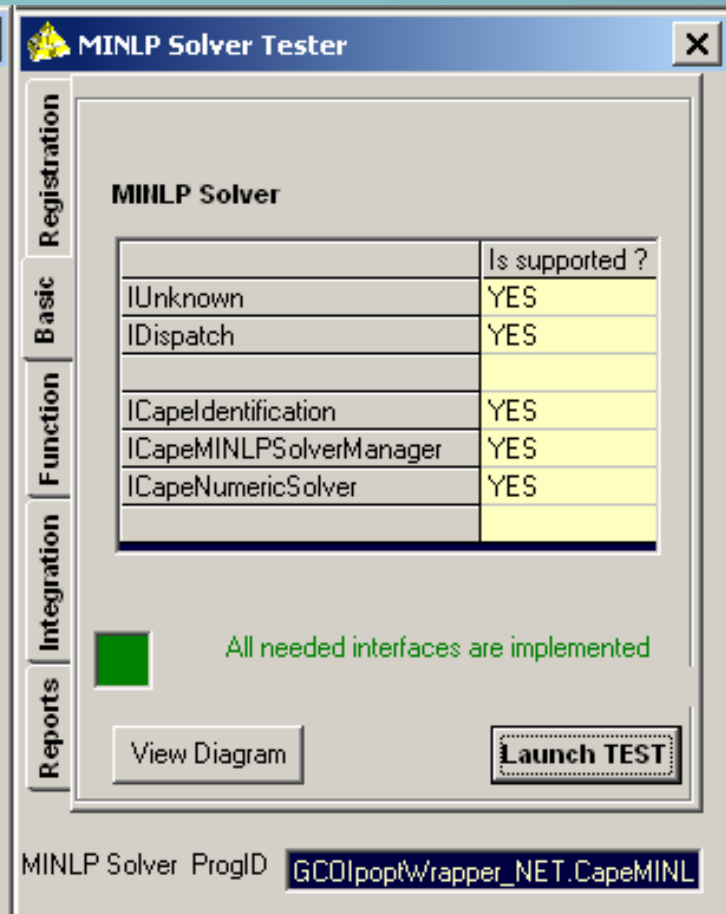
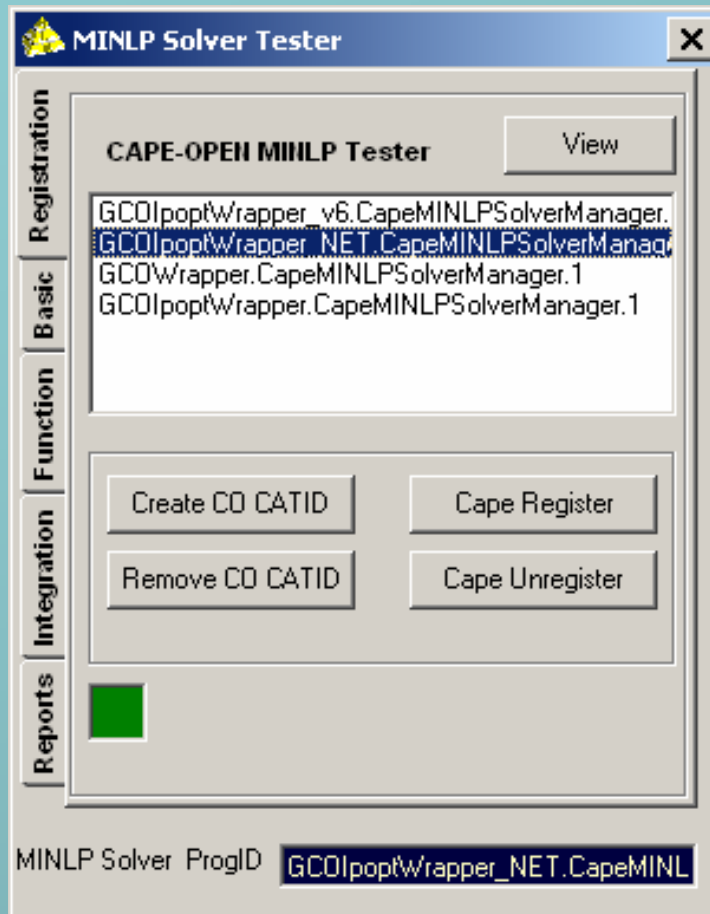
  

|    | X1 | X2 | X3 | Y1 | Y2 | Y3 | Log(X2+1) | Log(X1-X2+) | LB   | UB |
|----|----|----|----|----|----|----|-----------|-------------|------|----|
| C1 | 0  | 0  | -8 | 0  | 0  | 0  | 0.8       | 0.96        | -Inf | 0  |
| C2 | 0  | 0  | -1 | 0  | 0  | -2 | 1         | 1.2         | -Inf | 2  |
| C3 | -1 | 1  | 0  | 0  | 0  | 0  | 0         | 0           | -Inf | 0  |
| C4 | 0  | 1  | 0  | 1  | -2 | 0  | 0         | 0           | -Inf | 0  |
| C5 | 1  | -1 | 0  | 0  | -2 | 0  | 0         | 0           | -Inf | 0  |
| C6 | 0  | 0  | 0  | 1  | 1  | 0  | 0         | 0           | -Inf | 1  |

|            | X1    | X2    | X3    | Y1    | Y2    | Y3    |
|------------|-------|-------|-------|-------|-------|-------|
| Integer    | False | False | False | False | False | False |
| LowerBound | 2     | 0     | -Inf  | 0.1   | 0.2   | 0.3   |
| UpperBound | 4     | 2     | 3     | 1.1   | 1.2   | 1.3   |






**MINLP Solver Tester**

Registration Basic Function Integration Reports

**MINLP Solver**

|                         | Is supported ? |
|-------------------------|----------------|
| IUnknown                | YES            |
| IDispatch               | YES            |
|                         |                |
| ICapeIdentification     | YES            |
| ICapeMINLPSolverManager | YES            |
| ICapeNumericSolver      | YES            |
|                         |                |

 All needed interfaces are implemented

View Diagram Launch TEST

MINLP Solver ProgID **GCOIpopWrapper\_NET.CapeMINL**

**MINLP Solver Tester**

Registration Basic Function Integration Reports

**Solver Side** **Problem Side**

|                   | Is called ? |
|-------------------|-------------|
| CreateMINLPSystem | Yes         |
| Solve             | Yes         |
|                   |             |
|                   |             |
|                   |             |
|                   |             |
|                   |             |

Launch TEST

MINLP Solver ProgID **GCOIpopWrapper\_NET.CapeMINL**

**MINLP Solver Tester**

Registration | Basic | Function | Integration | Reports

**Solver Side** **Problem Side**

|                           | Counted calls |
|---------------------------|---------------|
| GetMINLPSize              | 2             |
| GetMINLPStructure         | 2             |
| GetMINLPVariableNames     | 0             |
| GetMINLPVariableTypes     | 2             |
| GetMINLPVariableBounds    | 2             |
| GetMINLPVariableValues    | 1             |
| SetMINLPVariableValues    | 81            |
| GetMINLPVariableBoolean   | 0             |
| GetMINLPVariableIntegerA  | 0             |
| GetMINLPVariableDoubleA   | 0             |
| GetMINLPVariableStringAtt | 0             |

**Launch TEST**

MINLP Solver ProgID **GCOIpop/wrapper\_NET.CapeMINL**

**MINLP Solver Tester**

Registration | Basic | Function | Integration | Reports

**Solver Side** **Problem Side**

|                          | Counted calls |
|--------------------------|---------------|
| GetMINLPNonlinearObjecti | 16            |
| GetMINLPObjectiveFunc    | 17            |
| GetMINLPObjectiveFunc    | 0             |
| GetMINLPObjectiveFunc    | 0             |
| GetMINLPObjectiveFunc    | 0             |
| GetMINLPObjectiveFunc    | 0             |
| SetMINLPLagrangeMultipli | 16            |
| GetMINLPLagrangeMultipli | 0             |
| SetMINLPHessianValues    | 16            |
| GetMINLPHessianStructure | 1             |
| GetMINLPHessianValues    | 16            |

**Launch TEST**

MINLP Solver ProgID **GCOIpop/wrapper\_NET.CapeMINL**

# Conclusions

- IPOPT is an efficient and well tested NLP solver
- IPOPT is freely available from [www.coin-or.org](http://www.coin-or.org) under a Common Public License (CPL)
- An interface has been developed to make IPOPT CAPE-OPEN compliant.
- As CAPE-OPEN MINLP compliant modeling systems become available, CO community will benefit from using IPOPT for solving large-scale NLP problems.

# Acknowledgements

- Dr. Michel Pons in CO-LaN offering the source code of MINLP tester.
- Dr. Antonio Espuna at UPC for helpful discussion.